Design Optimization of an Auto-Thermal Ammonia Synthesis Reactor Using Genetic Algorithm

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Abstract

This paper develops an improved harmony search (IHS) algorithm for the estimation of optimal length of reactor for different top temperatures with the constraints of energy and mass balance of reaction and feed gas temperature and mass flow rate of nitrogen for ammonia production. Thousands of combinations of feed gas temperature, nitrogen mass flow rate, reacting gas temperature and reactor length are possible. The new results obtained for an optimal reactor length and a top temperature are presented and compared to HS and other heuristic or deterministic methods. The results reveal that the proposed algorithm can find better solutions.

Keywords: *Improved harmony search; Ammonia synthesis reactor; Genetic algorithm; Optimization*

I. Introduction

Ammonia synthesis system is an important chemical process, in which the reactor is the key device, hence the necessity of its study so as to know the effects of operating parameters upon its performance. Mathematical models for simulation and optimization purpose have been developed and reported in the literature [1–4].
In the present work, the simulation was carried out using numerical techniques namely, Runge-Kutta method (fourth order) with fixed step size. [5]. Then the effect of top temperature on optimal reactor length was discussed. Genetic algorithm [6] was used for optimization along with Runge-Kutta (RK4) (with step size of 0.001) considering both top temperature and reactor length as the independent variables.

II. Problem Formulation

The Problem formulation is similar to that given in [1-3]. Feed gas contained 21.75 mole% nitrogen, 65.25 mole% hydrogen, 5 mole% ammonia, 4 mole% methane and 4 mole% argon. In a typical ammonia synthesis reactor, feed gas enters the reactor from the bottom. The yield of ammonia depends on the temperature of feed gas at the top of the reactor (henceforth called top temperature), the partial pressures of the reactants (nitrogen and hydrogen), and the reactor length. Figure 1 shows the schematic diagram of the ammonia reactor studied.

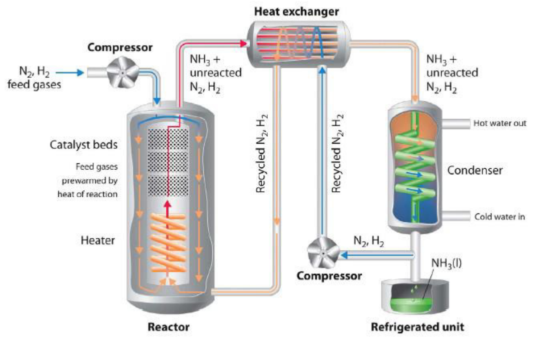

Figure 1. Schematic diagram of an ammonia reactor.

A. *Objective Function*

The objective function depicts the economic return based on the difference between the value of the product gas and the feed gas less the reactor capital cost return. A similar objective function for the process to that reported in [3] was adopted as:

$$F(x, N_{N2}, T_f, T_g) = 1.33563*10^7 - 1.70843*10^4 N_{N2} + 704,09(T_g - T_0) - 699.27(T_f - T_0) - [3.45663*10^7 + 1.98365*10^9 x]^{1/2} \quad (1)$$

It is clear from the above expression that the objective function depends on four variables: the reactor length (x), proportion of nitrogen (N_{N2}), the reacting gas temperature (Tg), and the feed gas temperature (T_f), for a given top temperature (T_0). The system model has three differential equations and four variables, hence a number of degrees of freedom equal to one. The length of the reactor was specified to calculate the remaining variables using the system model and then to transfer the obtained values to the optimization routine. The computation procedure for the carried out optimization is shown in Figure 2.

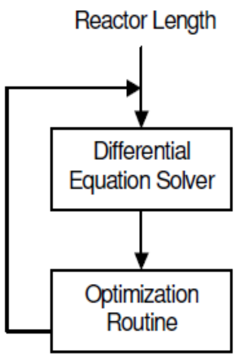

Figure.2. Computational procedures

B. Energy Balance Equations

Equations 2-6 are the energy balances that need to be satisfied in order to get the value of the three variables:

$$\frac{dT_f}{dx} = \frac{U.S_1}{W.C_{pf}}\left(T_g - T_f\right) \tag{2}$$

$$\frac{dT_g}{dx} = \frac{U.S_1}{W.C_{pg}}\left(T_g - T_f\right) + \frac{(-\Delta H)S_2}{W.C_{pg}}\left(\frac{dN_{N_2}}{dx}\right) \tag{3}$$

$$\frac{dN_{N_2}}{dx} = -f\left[k_1 \frac{p_{N_2} p_{H_2}^{1.5}}{p_{NH_3}} - k_2 \frac{p_{NH_3}}{p_{H_2}^{1.5}}\right] \tag{4}$$

Where

$$k_1 = 1.78954 \times 10^4 \exp\left(\frac{-20800}{RT_g}\right) \tag{5}$$

$$k_2 = 2.5714 \times 10^{16} \exp\left(\frac{-47400}{RT_g}\right) \tag{6}$$

C. Equality Constraints

The partial pressures that appear in the above energy equations are computed as shown by Equation 7:

$$p_{N_2} = \frac{286 N_{N_2}}{2.598 N_{N_{20}} + 2 N_{N_2}} \tag{7a}$$

$$p_{H_2} = 3 p_{N_2} \tag{7b}$$

$$p_{H_2} = 3 p_{N_2} \tag{7c}$$

The boundary conditions are:

$$T_f(x=0) = T_0 \;;\; T_g(x=0) = T_f \;; \tag{8a}$$

$$N_{N_2}(x=0) = 701.2 \frac{Kmol}{m^2.h} \tag{8b}$$

D. Inequality Constraints

The three inequality constraints that limit the values of three of the design variables are as given below:

$$\begin{gathered} 0 \le \frac{Kmol}{m^2.h} \le N_{N_2} \le 3220 \frac{Kmol}{m^2.h} \\ 400K \le T_f \le 800K \\ 0m \le x \le 10m \end{gathered} \tag{9}$$

Since the Reaction gas temperature (Tg) depends on the Nitrogen mass flow rate (N_{N2}), feed gas temperature (T_f) and reactor length (x), explicit boundaries on Tg are not necessary.

The software used for modeling was in MATLAB Version 6.1 and the method used to solve the objective function was Genetic Algorithm (GA).

III. Results and Discussions

Four MATLAB programming files and optimization tool Matlab were developed to model and optimize the ammonia reactor. From the obtained profiles shown in Figures 3 and 4, it was found out that the optimum reactor length was 6.695m and the corresponding objective function was 5.0168.106 $per year. The corresponding values of F, N_2, T_f and Tg are shown in the following table:

Table.1: Results obtained from optimization using ODE45-GA

X(m)	N_{N2}	T_f	T_g	***F*** (10^6 \$/y)
6.695	490.81	401.00	629.68	5.0168

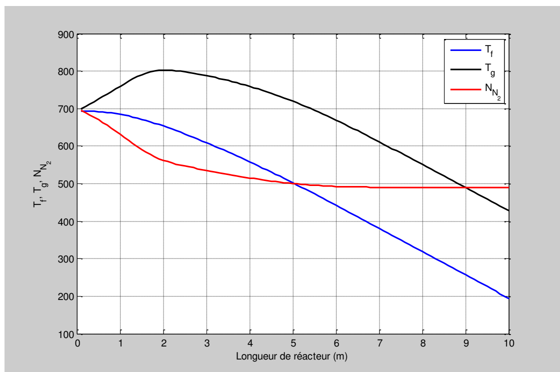

Figure. 3. Profiles of N_{N2}, T_f and T_g *vs* Reactor Length

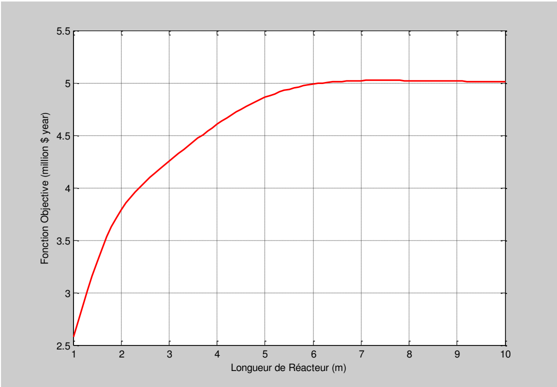

Figure. 4 Profiles of the objective function *vs* Reactor Length

IV. CONCLUSION

In the present study the genetic algorithm (GA) was used for the optimal design of an auto-thermal ammonia synthesis reactor. The results illustrated the accuracy and efficiency of the ODE-GA method for the solution of differential equations. The optimum reactor length depended upon the top temperature, at this temperature, the reactor length of 6.695m was found to give the optimum objective function value of $ 5,0168106 $/ year.

5. References

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